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ISSN 1463–9076 CODEN PPCPFQ 26(8) 6461–7242 (2024)

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Adventures in interdisciplinary science: a half century at the nexus between chemistry, physics and biology

Judith Herzfeld

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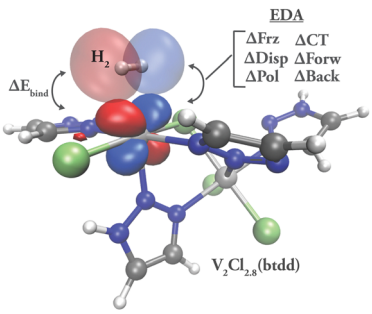
Quantum chemical modeling of hydrogen binding in metal–organic frameworks: validation, insight, predictions and challenges

Romit Chakraborty,* Justin J. Talbot, Hengyuan Shen, Yuto Yabuuchi, Kurtis M. Carsch, Henry Z. H. Jiang, Hiroyasu Furukawa, Jeffrey R. Long and Martin Head-Gordon*



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PERSPECTIVES

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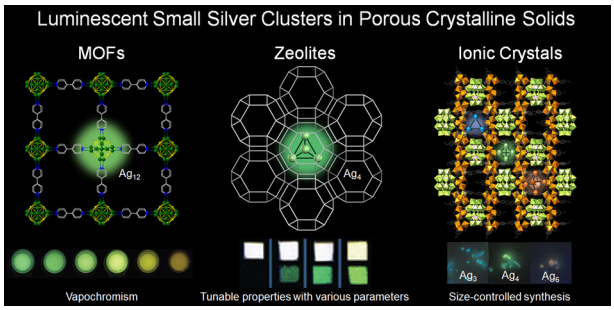
Small luminescent silver clusters stabilized in porous crystalline solids

Naoya Haraguchi, Taisei Kurosaki and Sayaka Uchida*



COMMUNICATION

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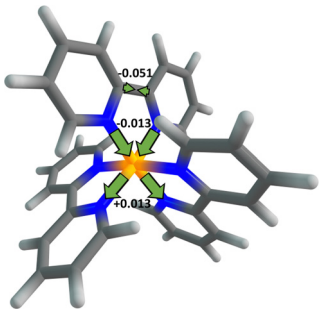
Nature of ultrafast dynamics in the lowest-lying singlet excited state of $[Ru(bpy)_3]^{2+}$

Chenyu Zeng, Yaqi Li, Hangjing Zheng, Mingxing Ren, Wei Wu and Zhenhua Chen*



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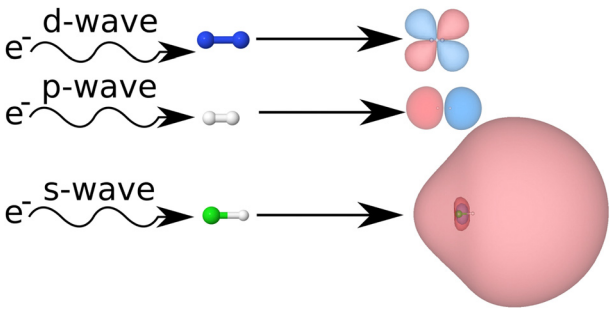
Signatures of s-wave scattering in bound electronic states

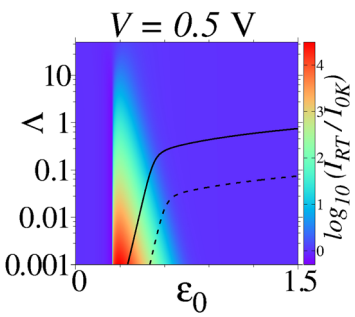
Robin E. Moorby,* Valentina Parravicini, Maristella Alessio and Thomas-C. Jagau*



6540

Can tunneling current in molecular junctions be so strongly temperature dependent to challenge a hopping mechanism? Analytical formulas answer this question and provide important insight into large area junctions

Ioan Bâldea



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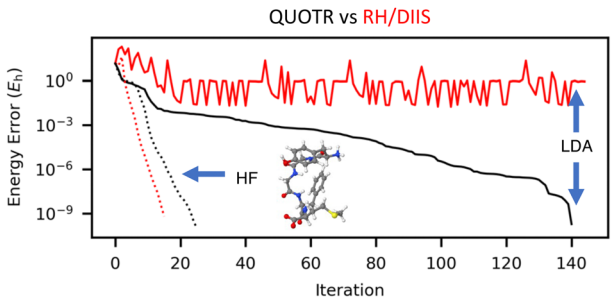

Economical quasi-Newton unitary optimization of electronic orbitals

Samuel A. Slattery, Kshitijkumar A. Surjuse, Charles C. Peterson, Deborah A. Penchoff and Edward F. Valeev*

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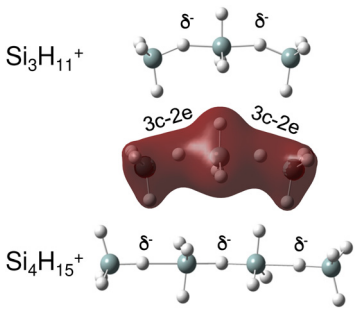

Infrared spectra of $Si_nH_{4n-1}^+$ ions (n = 2–8): inorganic H–$(Si–H)_{n-1}$ hydride wires of penta-coordinated Si in 3c–2e and charge-inverted hydrogen bonds

Martin Andreas Robert George and Otto Dopfer*

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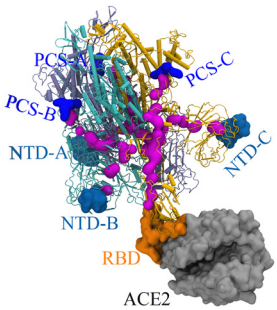

Allosteric regulation in SARS-CoV-2 spike protein

Yong Wei, Amy X. Chen, Yuewei Lin, Tao Wei* and Baofu Qiao*

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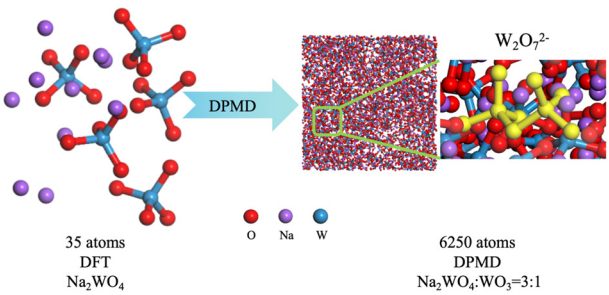

Effect of electric fields on tungsten distribution in Na_2WO_4–WO_3 molten salt

Yuliang Guo, Xiaobo Sun, Handong Jiao, Liwen Zhang, Wenxuan Qin, Xiaoli Xi* and Zuoren Nie*

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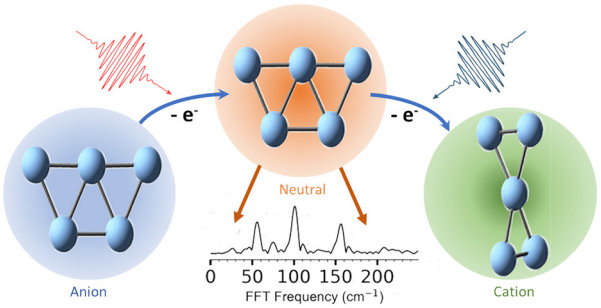
Vibrational wave-packet dynamics of the silver pentamer probed by femtosecond NeNePo spectroscopy

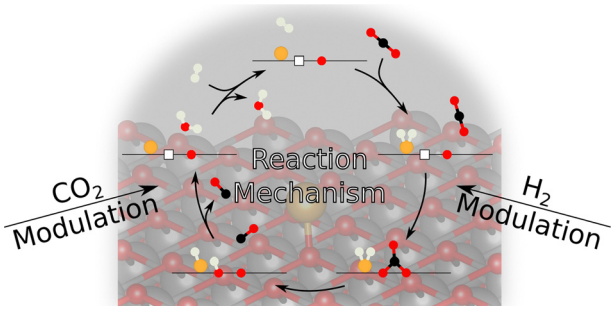
Max Grellmann, Martin DeWitt, Daniel M. Neumark, Knut R. Asmis and Jiaye Jin*



6608

Refining the mechanism of CO_2 and H_2 activation over gold-ceria catalysts by IR modulation excitation spectroscopy

Jakob Weyel and Christian Hess*



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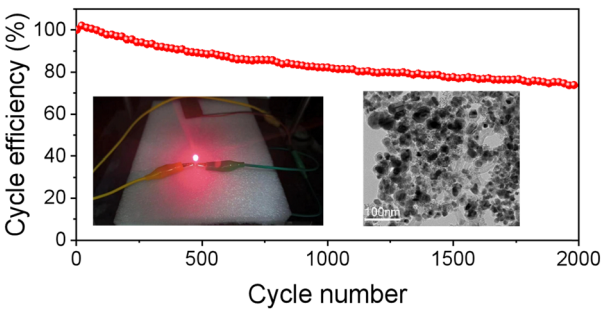
MOF-derived $NiAl_2O_4/NiCo_2O_4$ porous materials as supercapacitors with high electrochemical performance

Changyu Hu, Huidong Xie,* Yibo Wang, Hu Liu, Yajuan Zhao and Chang Yang



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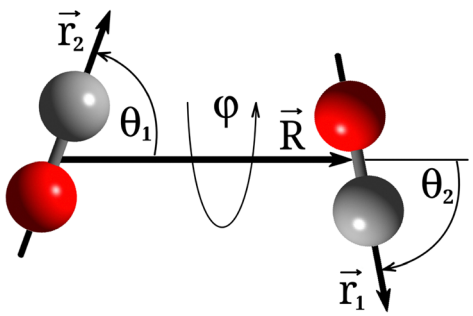
Mixed quantum/classical calculations of rotationally inelastic scattering in the CO + CO system: a comparison with fully quantum results

Dulat Bostan, Bikramaditya Mandal, Carolin Joy, Michał Żółtowski, François Lique, Jérôme Loreau, Ernesto Quintas-Sánchez, Adrian Batista-Planas, Richard Dawes and Dmitri Babikov*



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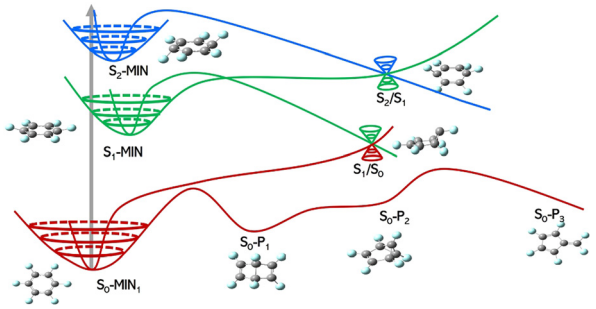

Photochemical mechanistic study of hexafluorobenzene involving the low-lying states

Duoduo Li, Xinli Song,* Jinming Liu and Song Zhang*

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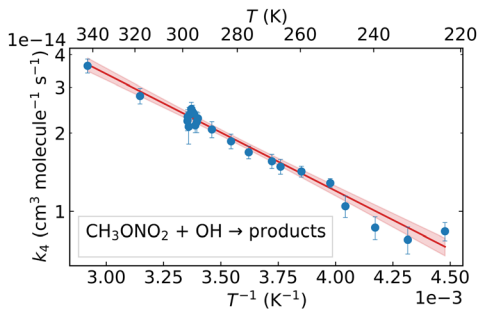

Kinetics of the reaction of OH with methyl nitrate (223–343 K)

Christin Fernholz, Fabienne Baumann, Jos Lelieveld and John N. Crowley*

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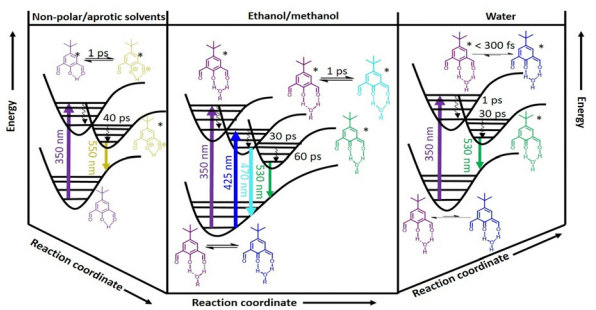

Non-trivial ground and excited state photophysics of a substituted phenol

Aparna Shukla, Vikas Kumar Jha and Soumit Chatterjee*

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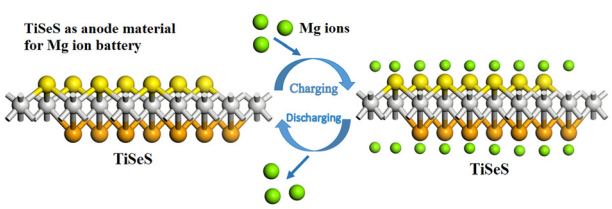

Exploring the anodic performance of ScSeS and TiSeS monolayers of modified transition metal dichalcogenides for Mg ion batteries *via* DFT calculations

Sharah Sami Rifah, Md. Sakib Zaman, Afiya Akter Piya and Siraj Ud Daula Shamim*

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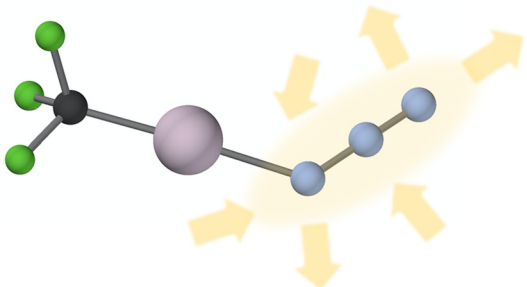
Planar tetracoordinate fluorine atom: global minimum with viable possibility

Kangkan Sarmah, Amlan J. Kalita and Ankur Kanti Guha*

6683

Azido-mediated intermolecular interactions of transition metal complexes

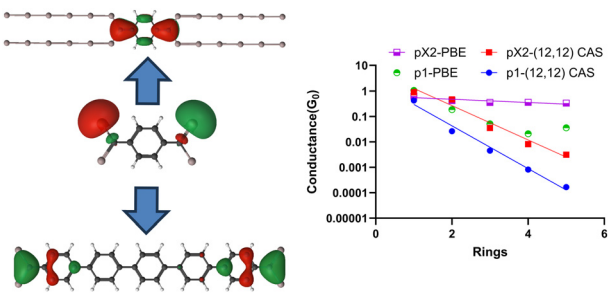
Juan D. Velasquez, Jorge Echeverría,*
Célia Fonseca Guerra* and Santiago Alvarez*



6696

Assessing the importance of multireference correlation in predicting reversed conductance decay

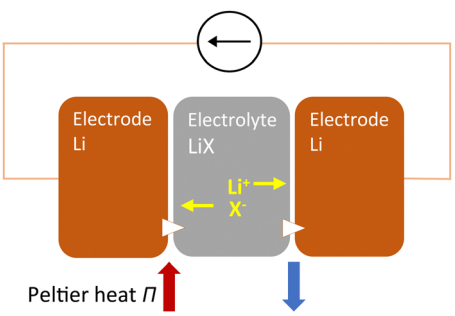
Tanner A. Cossaboon, Samir Kazmi, Matthew Tineo and Erik P. Hoy*



6708

Ionic Peltier effect in Li-ion electrolytes

Zhe Cheng, Yu-Ju Huang, Beniamin Zahiri, Patrick Kwon, Paul V. Braun and David G. Cahill*



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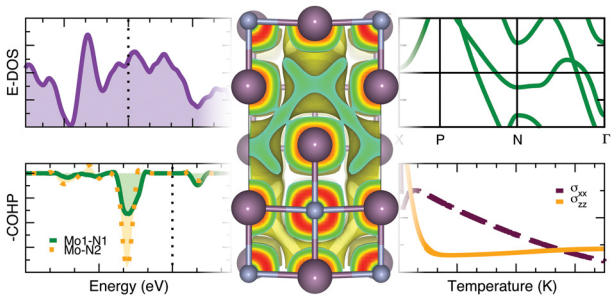
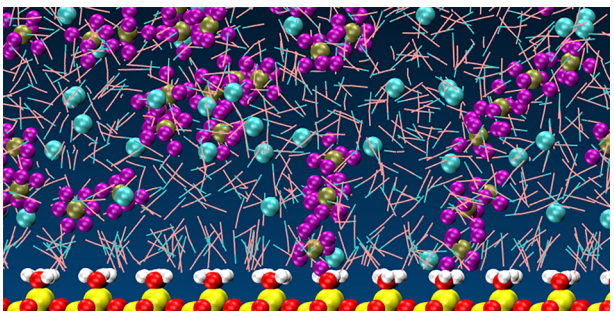


Metallicity and chemical bonding in anti-anatase Mo_2N

Lauren N. Walters and James M. Rondinelli*

6726



Beyond the electrical double layer model: ion-dependent effects in nanoscale solvent organization

Amanda J. Souna, Mohammad H. Motevaselian, Jake W. Polster, Jason D. Tran, Zuzanna S. Siwy, Narayana R. Aluru and John T. Fourkas*

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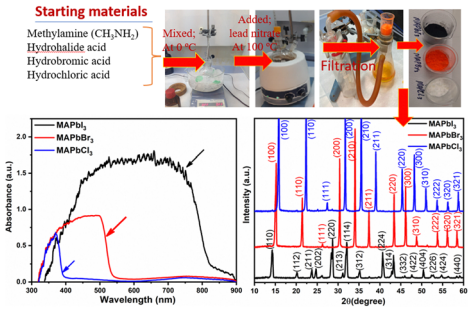

An intrinsic electrical conductivity study of perovskite powders $MAPbX_3$ (X = I, Br, Cl) to investigate its effect on their photovoltaic performance

Shafi Ullah,* Andreu Andrio, Julia Marí-Guaita, Hanif Ullah, Antonio Méndez-Blas, Roxana M. del Castillo Vázquez, Bernabé Mari and Vicente Compañ*

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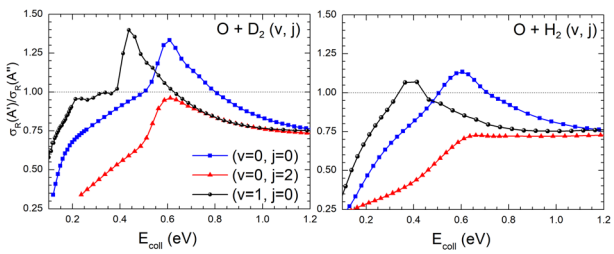

Dynamical effects on the $O(^3P) + D_2$ reaction and its impact on the Λ-doublet population

A. Veselinova, M. Menéndez, L. González-Sánchez, A. Zanchet, F. J. Aoiz and P. G. Jambrina*

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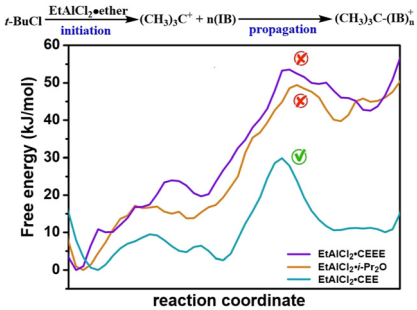
A theoretical study of the mechanism of cationic polymerization of isobutylene catalysed by $EtAlCl_2$/*t*-BuCl with bis(2-chloroethyl)ether in hexanes

Xinrong Yan, Meng Du, Jiwei Li, Ying Xue, Yibo Wu, Hao Zhang, Xin Wang* and Dingguo Xu*



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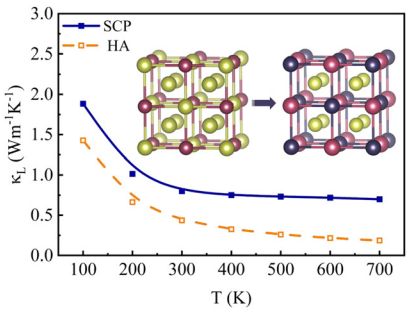
Novel room-temperature full-Heusler thermoelectric material Li_2TlSb

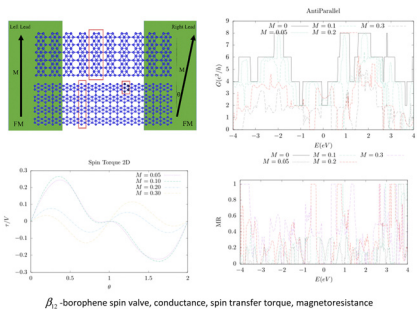
Siqi Guo, Jincheng Yue, Junda Li, Yanhui Liu* and Tian Cui*



6782

Spin-dependent transport and spin transfer torque in a borophene-based spin valve

Erfan Nikan* and Amirhossein Ahmadkhan Kordbacheh



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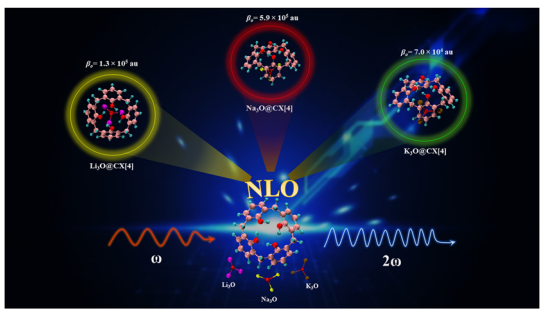
Unraveling the role of superalkalis in modulating the static and dynamic hyperpolarizabilities of emerging calix[4]arenes

Khalida Khalil, Shahnaz, Ralf Ludwig, Ammar M. Tighezza, Khurshid Ayub, Tariq Mahmood and Mazhar Amjad Gilani*



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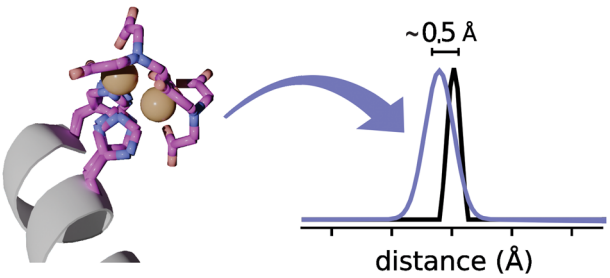
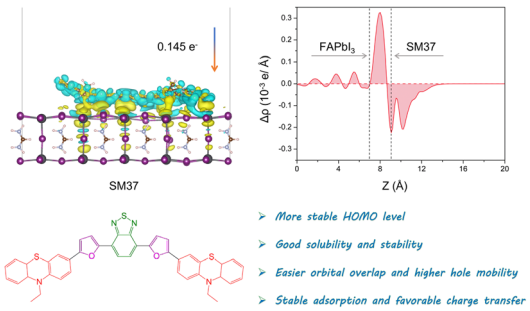


Modeling of Cu(II)-based protein spin labels using rotamer libraries

Zikri Hasanbasri, Maxx H. Tessmer, Stefan Stoll* and Sunil Saxena*

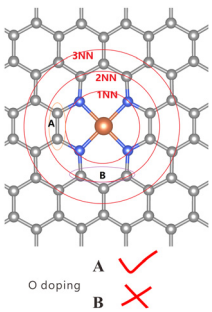
6817



Donor engineering of a benzothiadiazole-based D–A–D-type molecular semiconductor for perovskite solar cells: a theoretical study

Zhu-Zhu Sun,* Yushan Li* and Xing-Lei Xu

6826



The nearby atomic environment effect on an Fe–N–C catalyst for the oxygen reduction reaction: a density functional theory-based study

PengFei Yuan,* Chong Li, Jiannan Zhang, Fei Wang, Juanjuan Wang and Xuebo Chen*

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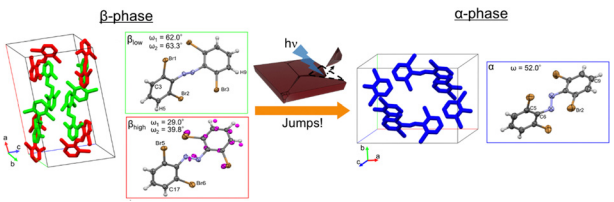

Releasing a bound molecular spring with light: a visible light-triggered photosalient effect tied to polymorphism

Keegan McGehee, Koichiro Saito, Dennis Kwaria, Hiroyuki Minamikawa and Yasuo Norikane*

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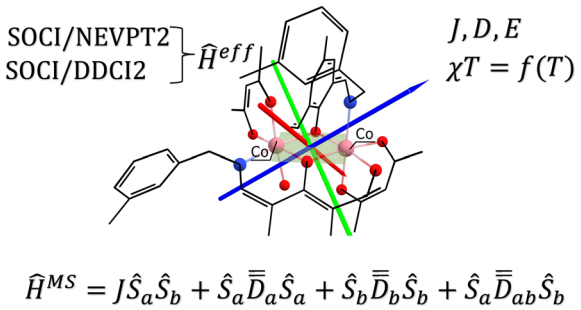
The resolution of the weak-exchange limit made rigorous, simple and general in binuclear complexes

Dumitru-Claudiu Sergentu, Boris Le Guennic and Rémi Maurice*



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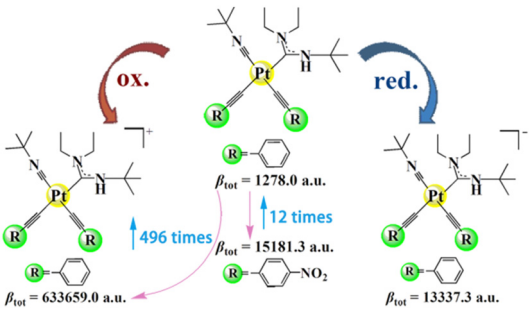
A theoretical study on the second-order nonlinear optical properties of Pt(II) bis-acetylide complexes: substituent and redox effects

Liting Sun, Yingying Wang, Yuanyuan Zhao* and Yongqing Qiu*



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Experimental and theoretical study of Criegee intermediate (CH_2OO) reactions with *n*-butyraldehyde and isobutyraldehyde: kinetics, implications and atmospheric fate

Amit Debnath and Balla Rajakumar*

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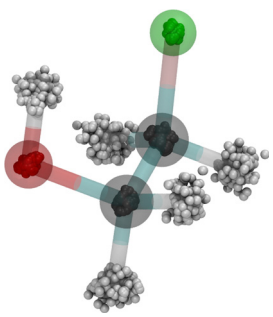
Nuclear quantum effects in gas-phase 2-fluoroethanol

Mrinal Arandhara and Sai G. Ramesh*



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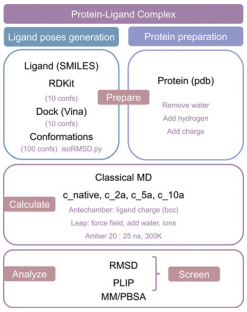
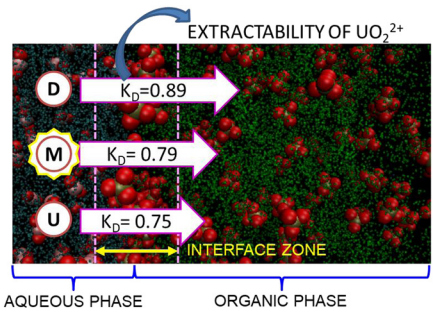


Elucidation of protein–ligand interactions by multiple trajectory analysis methods

Nian Wu,* Ruotian Zhang, Xingang Peng, Lincan Fang, Kai Chen and Joakim S. Jestilä

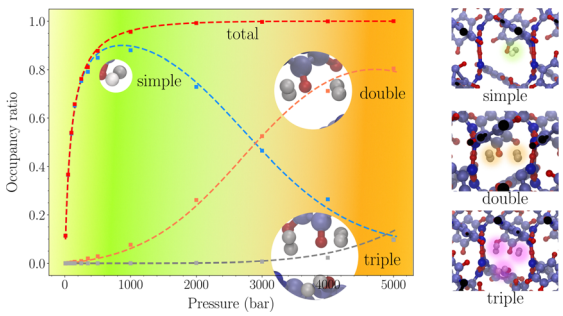
6916



Structure and dynamics of dissociated and undissociated forms of nitric acid and their implications in interfacial mass transfer: insights from molecular dynamics simulations

Arya Das and Sk. Musharaf Ali*

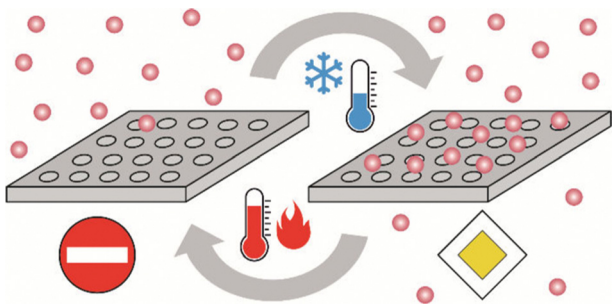
6939



Upper storage-capacity limit and multiple occupancy phenomena in H_2-hydroquinone clathrates using Monte Carlo and DFT simulations

B. Parage, C. Miqueu, M. Pérez-Rodríguez, T. Méndez-Morales and M. M. Piñeiro*

6949



Anti-Arrhenius passage of gaseous molecules through nanoporous two-dimensional membranes

Petr Dementyev* and Armin Gölzhäuser

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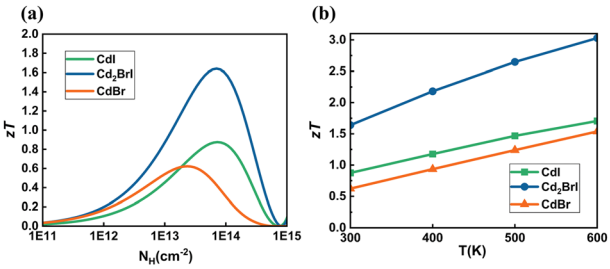
6956

The thermoelectric properties of CdBr, CdI, and Janus Cd_2BrI monolayers with low lattice thermal conductivity

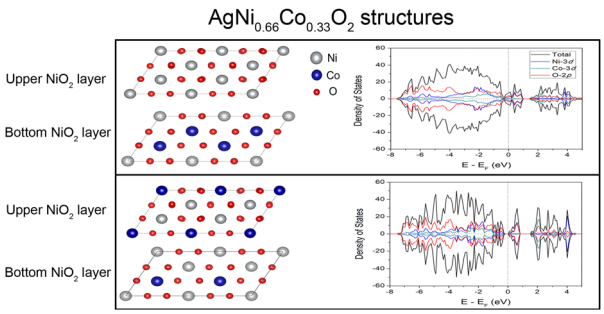
Yan-Ling Wu, Qiu Yang, Hua-Yun Geng and Yan Cheng*



6967

DFT+*U* and quantum Monte Carlo study of electronic and optical properties of $AgNiO_2$ and $AgNi_{1-x}Co_xO_2$ delafossite

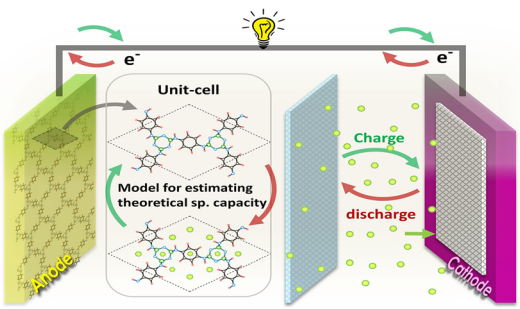
Hyeondeok Shin,* Panchapakesan Ganesh, Paul R. C. Kent, Anouar Benali, Anand Bhattacharya, Ho Nyung Lee, Olle Heinonen and Jaron T. Krogel*



6977

Enhanced As-COF nanochannels as a high-capacity anode for K and Ca-ion batteries

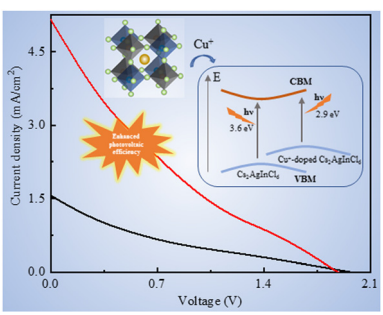
Shehzad Ahmed, Awais Ghani, Imran Muhammad, Iltaf Muhammad, Andleeb Mehmood, Naeem Ullah, Arzoo Hassan, Yong Wang, Xiaoqing Tian* and Boris Yakobson



6984

Cu^+-doped lead-free double perovskite quantum dots for enhancing the photovoltaic performance of carbon-based $Cs_2AgInCl_6$ perovskite solar cells

Yanting Li, Jiaying Li, Sidi Ye, Yanting Liu, Lili Meng, Hua Yao and Qian Chen*



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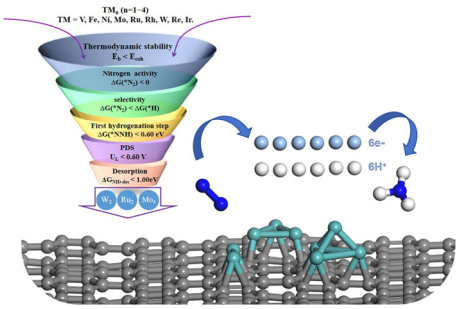
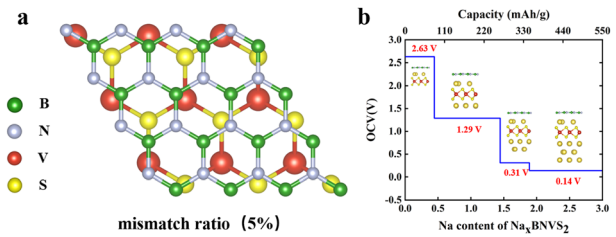
6991



Transition metal small clusters anchored on biphenylene for effective electrocatalytic nitrogen reduction

Yan Gao, Qingchen Li, Zhilii Yin, Haifeng Wang,* Zhong Wei* and Junfeng Gao*

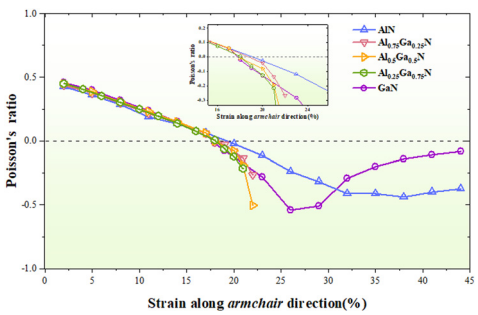
7001



Theoretical insights into the intercalation mechanism of Li, Na, and Mg ions in a metallic BN/VS_2 heterostructure

Lingxiao Luo, Shuangshuang Tan,* Zhipeng Gao, Xiaofang Yang,* Junyao Xu,* Guangsheng Huang, Jingfeng Wang and Fusheng Pan

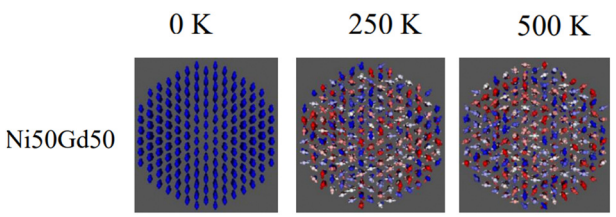
7010



Alloying enhanced negative Poisson's ratio in two-dimensional aluminum gallium nitride ($Al_xGa_{1-x}N$)

Xiaoxia Wang, Zhunyun Tang, Linfeng Yu, Donghai Wei, Zonghao Yuan, Chao Tang, Huimin Wang,* Tao Ouyang* and Guangzhao Qin*

7020



Exploring intermixed magnetic nanoparticles: insights from atomistic spin dynamics simulations

Junais Habeeb Mokkath,* Remya Nair and Mufasila Mumthaz Muhammed

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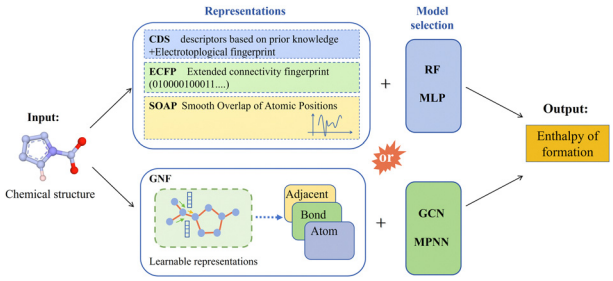
7029

Predicting the enthalpy of formation of energetic molecules *via* conventional machine learning and GNN

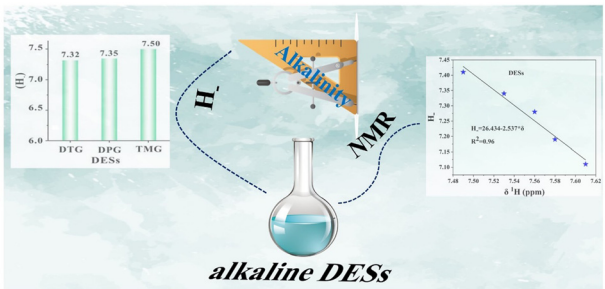
Di Zhang, Qingzhao Chu and Dongping Chen*



7042

Quantification of alkalinity of deep eutectic solvents based on (H_) and NMR

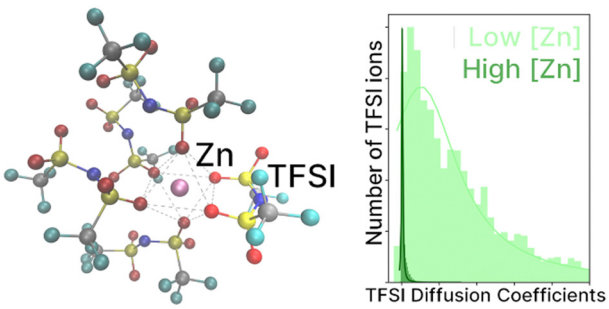
Rui Qin, Zeyu Wang, Chenyang Wei, Fengyi Zhou, Yurun Tian, Yu Chen* and Tiancheng Mu*



7049

Impact of Li, Na and Zn metal cation concentration in EMIM–TFSI ionic liquids on ion clustering, structure and dynamics

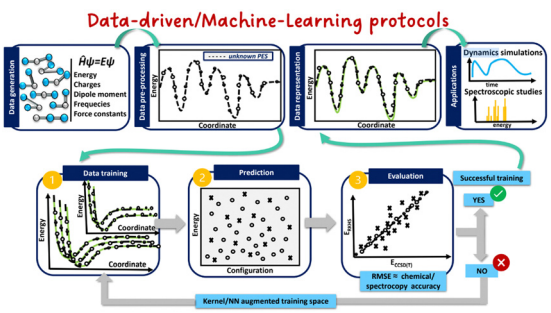
Samanvitha Kunigal Vijaya Shankar, Yann Claveau,* Tojo Rasoanarivo, Chris Ewels and Jean Le Bideau



7060

A kernel-based machine learning potential and quantum vibrational state analysis of the cationic Ar hydride (Ar_2H^+)

María Judit Montes de Oca-Estévez, Álvaro Valdés and Rita Prosmiti*



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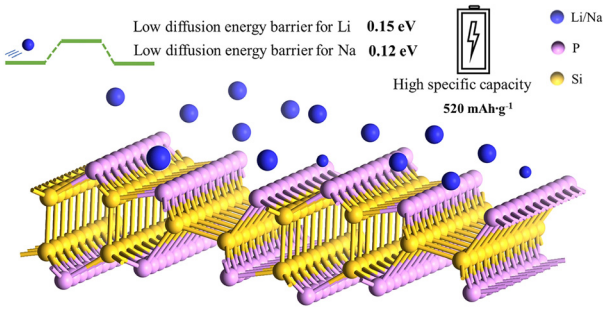
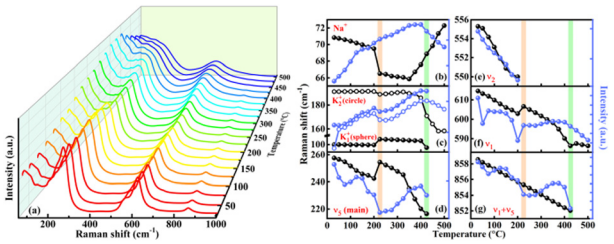
7072



A first-principles study of 2D single-layer SiP as anode materials for lithium-ion batteries and sodium-ion batteries

Yingying Xing, Chihao Cao, Zhong Huang, Liang Huang,* Haijun Zhang* and Quanli Jia

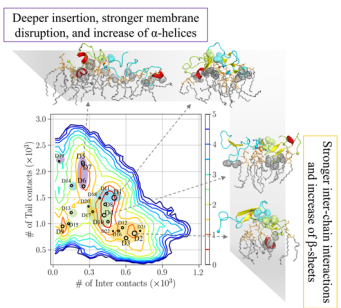
7083



Deciphering the *in situ* phonon evolution of potassium sodium niobate under varying temperature and electric fields

L. G. Wang, Y. S. Wang, C. M. Zhu,* M. Y. Qin, J. Y. Wei and Y. Jiang*

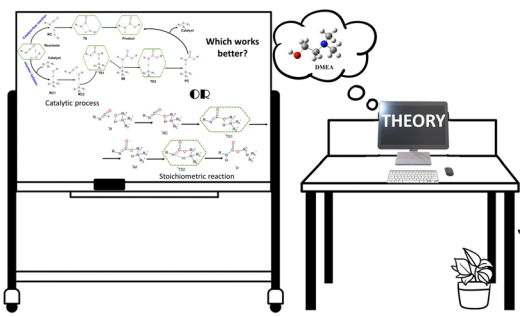
7090



Structural diversity in the membrane-bound hIAPP dimer correlated with distinct membrane disruption mechanisms

Qin Qiao,* Guanghong Wei and Zhijian Song

7103



Stoichiometric reaction and catalytic effect of 2-dimethylaminoethanol in urethane formation

Hadeer Q. Waleed, Rachid Hadjadj, Béla Viskolcz and Béla Fiser*

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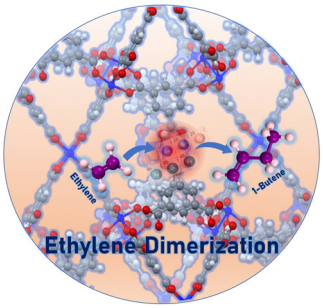
7109

Computational design of metal hydrides on a defective metal–organic framework HKUST-1 for ethylene dimerization

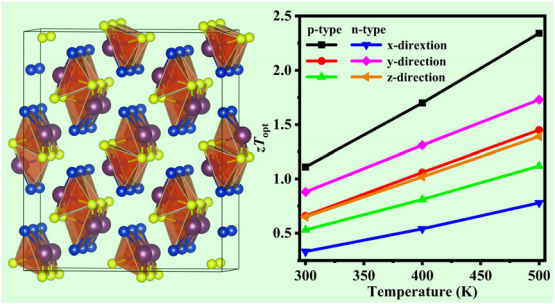
Karam Hashem, Ramakrishna Krishnan, Kuiwei Yang, Bai Amutha Anjali, Yugen Zhang and Jianwen Jiang*



7124

One-dimensional van der Waals BiSBr: an anisotropic thermoelectric mineral

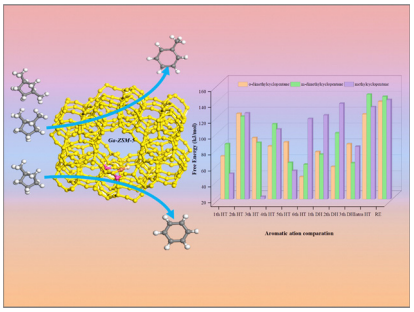
Prakash Govindaraj, Kowsalya Murugan and Kathirvel Venugopal*



7137

A density functional theory study on the mechanism of toluene from dimethylcyclopentane catalyzed by the $[GaH]^{2+}$ active site of Ga-ZSM-5

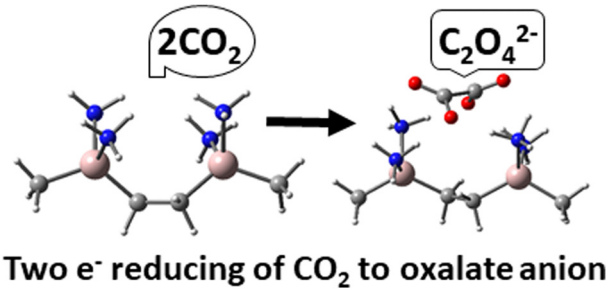
Hongyan Liu, Furong Sun, Junzhuo Xu, Hairong Zhang,* Tingting Wu, Shenghua Han, Shijun Zhang, Yan Mo, Lixia Ling, Riguang Zhang, Maohong Fan* and Baojun Wang*



7149

A two-electron reducing reaction of CO_2 to an oxalate anion: a theoretical study of delocalized (presolvated) electrons in $Al(CH_3)_n(NH_3)_m$, n = 0–2 and m = 1–6, clusters

Mohammad Esmail Alikhani* and Benjamin G. Janesko



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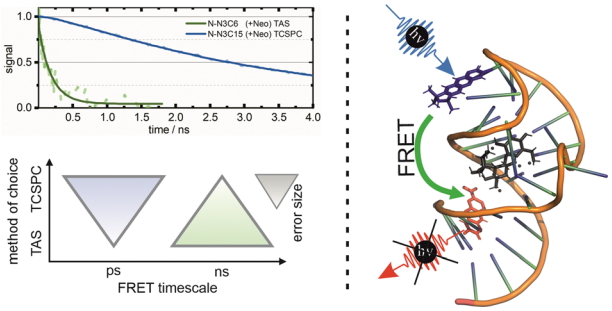
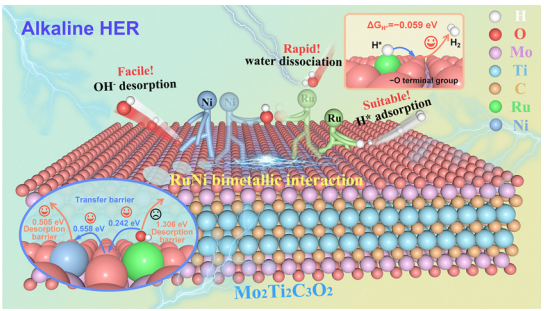


Förster resonance energy transfer within the neomycin aptamer

Florian Hurter, Anna-Lena J. Halbritter, Iram M. Ahmad, Markus Braun, Snorri Th. Sigurdsson and Josef Wachtveitl*

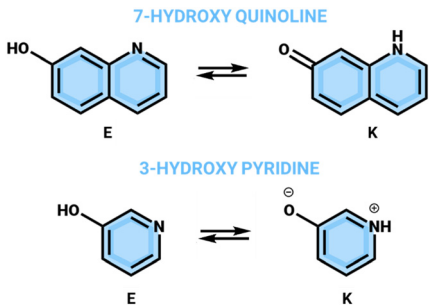
7166



NiRu–$Mo_2Ti_2C_3O_2$ as an efficient catalyst for alkaline hydrogen evolution reactions: the role of bimetallic site interactions in promoting Volmer-step kinetics

Qing Xi, Fangxia Xie, Zijun Sun, Jianxin Liu, Xiaochao Zhang, Yawen Wang, Aijuan Zhou, Xiaoli Ma,* Xiaoming Gao, Xiuping Yue, Jun Ren, Caimei Fan, Xuan Jian and Rui Li*

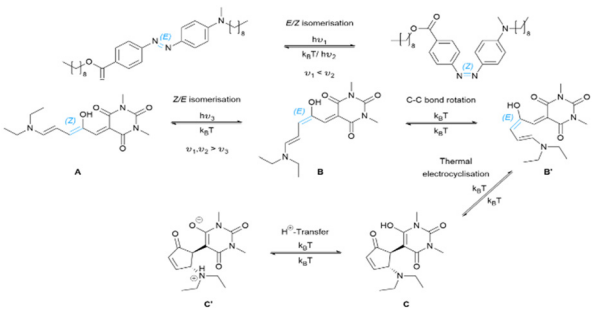
7177



Azaindolizine proton cranes attached to 7-hydroxyquinoline and 3-hydroxypyridine: a comparative theoretical study

Sofia Slavova and Liudmil Antonov*

7190



Characteristics and long-term kinetics of an azobenzene derivative and a donor–acceptor Stenhouse adduct as orthogonal photoswitches

Tanja Schmitt, Christian Huck, Nils Oberhof, Li-Yun Hsu, Eva Blasco, Andreas Dreuw and Petra Tegeder*

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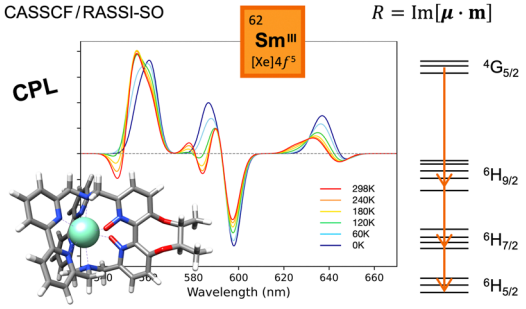
7203

Ab initio investigations of circularly polarised luminescence in Samarium(III)-based complexes

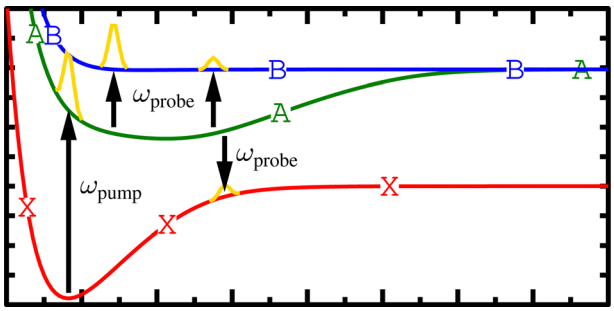
Maxime Grasser and Boris Le Guennic*



7211

Light-induced photodissociation in the lowest three electronic states of the NaH molecule

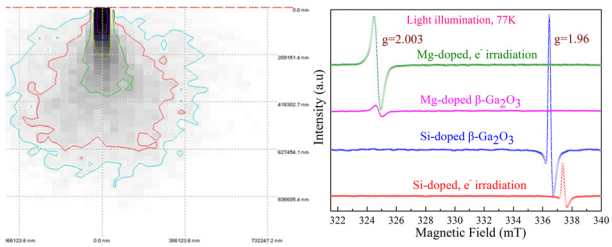
Otabek Umarov, András Csehi, Péter Badankó, Gábor J. Halász and Ágnes Vibók*



7224

Impact of electron irradiation on semi-insulating and conductive β-Ga_2O_3 single crystals

Jinpeng Lv,* Lingzhe Ren and Yubao Zhang

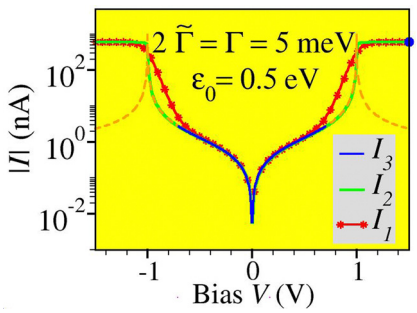


COMMENTS

7230

Comment on "A single level tunneling model for molecular junctions: evaluating the simulation methods" by E. M. Opodi, X. Song, X. Yu and W. Hu, _Phys. Chem. Chem. Phys._, 2022, 24, 11958"

Ioan Bâldea



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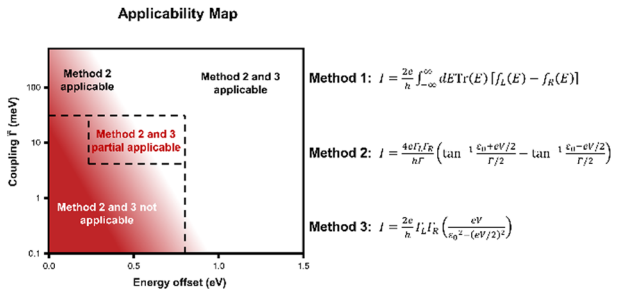
COMMENTS

7236



Reply to the 'Comment on "A single level tunneling model for molecular junctions: evaluating the simulation methods"' by I Baldea, *Phys. Chem. Chem. Phys.*, 2024, 26, D2CP05110A (http://D2CP05110A)

Zheyang Li and Xi Yu*

CORRECTION

7239

Correction: Impact of temperature-dependent non-PAN peroxynitrate formation, RO_2NO_2, on nighttime atmospheric chemistry

Michelle Färber, Luc Vereecken, Hendrik Fuchs, Georgios I. Gkatzelis, Franz Rohrer, Sergej Wedel, Andreas Wahner and Anna Novelli*

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